## **Multiclass Classification**

## Solution 1: Multiclass Hinge Loss

(a) We want to show that

$$L_{0-1}(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}} \le L(y, f(\mathbf{x})) = \max_{k} \left( f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbb{1}_{\{y \neq k\}} \right),$$

where

$$\mathcal{H} = \{ f = (f_1, \dots, f_g)^\top : \mathcal{X} \to \mathbb{R}^g \mid f_k : \mathcal{X} \to \mathbb{R}, \ \forall k \in \mathcal{Y} \}.$$

and

$$h(\mathbf{x}) = \arg\max_{k \in \{1, \dots, q\}} f_k(\mathbf{x}). \tag{1}$$

We distinguish two cases for any arbitrary data point pair  $(\mathbf{x}, y) \in \mathcal{X} \times \mathcal{Y}$ .

Case 1:  $h(\mathbf{x}) \neq y$ 

Thus,  $L_{0-1}(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}} = 1$  and in light of (1) this means that  $y \neq \arg\max_{k \in \{1, \dots, g\}} f_k(\mathbf{x})$ , so that there exists some  $\tilde{k} \neq y$  with  $f_{\tilde{k}}(\mathbf{x}) \geq f_y(\mathbf{x})$ .

$$L(y, f(\mathbf{x})) = \max_{k} \left( f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbbm{1}_{\{y \neq k\}} \right)$$
 (Definition) 
$$\geq \left( \underbrace{f_{\tilde{k}}(\mathbf{x}) - f_y(\mathbf{x})}_{\geq 0} + \mathbbm{1}_{\{y \neq \tilde{k}\}} \right)$$
 (max always greater than one single component) 
$$\geq \mathbbm{1}_{\{y \neq \tilde{k}\}}$$
 ( $f_{\tilde{k}}(\mathbf{x}) \geq f_y(\mathbf{x})$ ) 
$$= 1.$$
 (Indicator function is true)

Case 2:  $h(\mathbf{x}) = y$ 

Thus,  $L_{0-1}(y, h(\mathbf{x})) = \mathbb{1}_{\{y \neq h(\mathbf{x})\}} = 0$ . But it always holds that

$$\begin{split} L(y,f(\mathbf{x})) &= \max_{k} \left( f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbbm{1}_{\{y \neq k\}} \right) \\ &\geq \left( f_y(\mathbf{x}) - f_y(\mathbf{x}) + \mathbbm{1}_{\{y \neq y\}} \right) \\ &= \mathbbm{1}_{\{y \neq y\}} \\ &= 0. \end{split} \qquad \text{(Indicator function is not true)}$$

(b) For sake of convenience, define  $g_{k,y}(\mathbf{x}) = f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbb{1}_{\{y \neq k\}}$  for any  $k, y \in \mathcal{Y}$  and  $\mathbf{x} \in \mathcal{X}$ . If k = y, then of course  $g_{k,y}(\mathbf{x}) = 0$ , so that in order to find the maximum of the multiclass hinge loss, we need to check for each  $k \neq y$  whether  $g_{k,y}(\mathbf{x}) > 0$  holds. If this doesn't hold for any  $k \neq y$ , then the maximum is  $0 = g_{y,y}(\mathbf{x})$ . Thus,

$$L(y, f(\mathbf{x})) = \max_{k} \left( f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbb{1}_{\{y \neq k\}} \right)$$
 (Definition)  

$$= \max_{k} g_{k,y}(\mathbf{x})$$
 (Definition of  $g_{k,y}(\mathbf{x})$ )  

$$= \max_{k \neq y} \left( \max\{g_{y,y}(\mathbf{x}), g_{k,y}(\mathbf{x})\} \right)$$
 (Idea above)  

$$= \max_{k \neq y} \left( \max\{0, f_k(\mathbf{x}) - f_y(\mathbf{x}) + \mathbb{1}_{\{y \neq k\}}\} \right)$$
 (Definition of the  $g$ 's)  

$$= \max_{k \neq y} \left( \max\{0, f_k(\mathbf{x}) - f_y(\mathbf{x}) + 1\} \right)$$
 (Indicator function is true)  

$$\leq \sum_{k \neq y} \max\{0, f_k(\mathbf{x}) - f_y(\mathbf{x}) + 1\}.$$

(max is at most the sum over all the **non-negative** components)

(c) In the case of binary classification, i.e., g = 2 and  $\mathcal{Y} = \{-1, +1\}$ , we use a single discriminant model  $f(\mathbf{x}) = f_1(\mathbf{x}) - f_{-1}(\mathbf{x})$  based on two scoring functions  $f_1, f_{-1} : \mathcal{X} \to \mathbb{R}$  for the prediction by means of  $h(\mathbf{x}) = \operatorname{sgn}(f(\mathbf{x}))$ . Here,  $f_1$  is the score for the positive class and  $f_{-1}$  is the score for the negative class. Show that the upper bound in (b) coincides with the binary hinge loss  $L(y, f(\mathbf{x})) = \max\{0, 1 - yf(\mathbf{x})\}$ .

We distinguish two cases for  $y \in \mathcal{Y} = \{-1, +1\}.$ 

Case 1: y = +1

Then,

$$\sum_{k \neq y} \max\{0, f_k(\mathbf{x}) - f_y(\mathbf{x}) + 1\} = \sum_{k \neq +1} \max\{0, f_k(\mathbf{x}) - f_1(\mathbf{x}) + 1\}$$
 (Case  $y = +1$ )
$$= \max\{0, f_{-1}(\mathbf{x}) - f_1(\mathbf{x}) + 1\}$$
 (Binary classification, i.e.,  $k$  can only be  $-1$ )
$$= \max\{0, 1 - f(\mathbf{x})\}$$
 (Definition of  $f$ )
$$= \max\{0, 1 - yf(\mathbf{x})\}.$$
 (Case  $y = +1$ )

Case 2: y = -1

Then,

$$\sum_{k \neq y} \max\{0, f_k(\mathbf{x}) - f_y(\mathbf{x}) + 1\} = \sum_{k \neq -1} \max\{0, f_k(\mathbf{x}) - f_{-1}(\mathbf{x}) + 1\}$$
 (Case  $y = -1$ )
$$= \max\{0, f_1(\mathbf{x}) - f_{-1}(\mathbf{x}) + 1\}$$
 (Binary classification, i.e.,  $k$  can only be  $+1$ )
$$= \max\{0, 1 + f(\mathbf{x})\}$$
 (Definition of  $f$ )
$$= \max\{0, 1 - yf(\mathbf{x})\}.$$
 (Case  $y = -1$ )

(d) Yes, we can say something similar for the alternative multiclass hinge loss, namely that it is only zero if all the g-1 margins are greater or equal 1, where the margins are  $m_{y,k}(\mathbf{x}) = f_y(\mathbf{x}) - f_k(\mathbf{x})$  (y is the true class and  $k \in \mathcal{Y} \setminus \{y\}$ ). Indeed, it holds that

$$m_{y,k}(\mathbf{x}) \ge 1 \quad \forall k \ne y \quad \Leftrightarrow \quad f_y(\mathbf{x}) - f_k(\mathbf{x}) \ge 1 \quad \forall k \ne y$$

$$\Leftrightarrow \quad f_k(\mathbf{x}) - f_y(\mathbf{x}) \le -1 \quad \forall k \ne y$$

$$\Leftrightarrow \quad \max\{0, 1 + f_k(\mathbf{x}) - f_y(\mathbf{x})\} = 0 \quad \forall k \ne y$$

$$\Leftrightarrow \quad \sum_{k \ne y} \max\{0, 1 + f_k(\mathbf{x}) - f_y(\mathbf{x})\} = 0$$

(e) An empirical risk minimization approach for the (alternative) multiclass hinge loss will try to minimize the g-1 margins simultaneously, while the empirical risk minimization approach with the one-vs-rest technique will try to minimize the (binary) margins of the individual binary hinge losses separately. In particular, a model obtained by the former will in general not coincide with a model obtained by the latter approach. As an example we can consider the **iris** dataset:

```
return (1)
 else{
   return (-1)
# binary hinge loss for linear score function (characterized by theta)
bin_hinge <- function(z,theta){</pre>
 x = z[1:p]
 y = z[p+1]
 return(max(0,1-y*x%*%t(t(theta))))
# empirical risk for binary hinge loss for linear score function (characterized by theta)
emp_risk_bin_hinge <- function(Z,theta){</pre>
 sum(apply(Z,1,bin_hinge,theta=theta))
# fitting a linear score function in a one-vs-all manner
one_vs_all_bin_theta <-function(Z){</pre>
 theta_mat
            = matrix(rep(0,p*g),nrow=p)
 for(i in 1:g){
   # recode the last column of the data matrix according to the codebook
                = cbind(Z[,1:p], unlist(sapply(Z[,p+1],codebook,i)))
   # finding the best theta
   theta_mat[,i] = optim(rep(0,p),fn=emp_risk_bin_hinge,Z=Z_coded)$par
 return ( theta_mat )
# predication with linear score functions in a one-vs-all manner
# hat_theta_mat stores the parameters of the binary classifiers
one_vs_all_bin_predict <- function(hat_theta_mat,x){</pre>
 scores = x %*% hat_theta_mat
 return (which(scores==max(scores)))
# multiclass hinge loss for linear score functions (characterized by the matrix Theta)
multiclass_hinge<-function(z,Theta){</pre>
 Theta = matrix(Theta,nrow=p,byrow=T)
        = z[1:p]
        = z[p+1]
 temp = -1 # we start with -1, as in the for loop below we do not leave out the case k=y
 for(i in 1:g){
   temp = temp + \max(0, 1 + \text{Theta}[,i]\% *\% t(t(x)) - \text{Theta}[,y]\% *\% t(t(x)))
 }
 return(temp)
 # alternative if you do not like for-loops
 \#return (sum(pmax(rep(0,g), 1+ t(x))**Theta - as.numeric(Theta[,y])**t(t(x))))-1)
# empirical risk for multiclass hinge loss for linear score functions
# characterized by the matrix Theta
```

```
emp_risk_mutliclass_hinge <- function(Z,Theta){</pre>
  sum(apply(Z,1,multiclass_hinge,Theta=Theta))
# fitting linear score functions for multiclass hinge loss
mutliclass_hinge_theta <-function(Z){</pre>
  return ( optim(par=rep(0,p*g),fn=emp_risk_mutliclass_hinge,Z=Z)$par)
# predication with linear score functions for multiclass hinge loss
# hat_Theta is the fitted parameter matrix
mutliclass_hinge_predict <-function(hat_Theta,x){</pre>
 scores = x %*% hat_Theta
 return (which(scores==max(scores)))
# split the iris data into training and test data sets
set.seed(5)
train_ind <- sort(sample(1:nrow(Z),size=50,replace=F))</pre>
test_ind <-(1:150)[-train_ind]
# fit the parameters
hat_theta_mat <- one_vs_all_bin_theta(Z[train_ind,])</pre>
hat_Theta <- matrix(mutliclass_hinge_theta(Z[train_ind,]),nrow=p,byrow=T)</pre>
hat_Theta
##
              [,1]
                         [,2]
                                    [,3]
## [1,] -0.3501875 0.7707322 -0.3670786
## [2,] 0.1562045 0.3336436 -1.5647621
## [3,] 7.1427582 -2.3870077 -2.9751341
## [4,] -8.1156339 0.1446330 1.4809487
## [5,] 0.2199560 0.1785929 5.3625162
# counting how many times the predictions coincide
count = 0
for(j in test_ind){
  # if predictions differ, print the different predictions and the true label
  if(one_vs_all_bin_predict(hat_theta_mat,Z[j,1:p])!=
    mutliclass_hinge_predict(hat_Theta,Z[j,1:p])){
    print(paste("One_vs_all predicts: ",
                one_vs_all_bin_predict(hat_theta_mat,Z[j,1:p])))
    print(paste("Multiclass hinge loss predicts: ",
                mutliclass_hinge_predict(hat_Theta,Z[j,1:p])))
    print(paste("True label: ",Z[j,p+1]))
   print("")
  else{
    count <- count +1
## [1] "One_vs_all predicts: 2"
## [1] "Multiclass hinge loss predicts: 3"
## [1] "True label: 2"
```

```
## [1] ""
## [1] "One_vs_all predicts: 3"
## [1] "Multiclass hinge loss predicts: 2"
## [1] "True label: 2"
## [1] ""
## [1] "One_vs_all predicts: 3"
## [1] "Multiclass hinge loss predicts: 2"
## [1] "True label: 2"
## [1] ""
## [1] "One_vs_all predicts: 2"
## [1] "Multiclass hinge loss predicts: 3"
## [1] "True label: 3"
## [1] ""
## [1] "One_vs_all predicts: 2"
## [1] "Multiclass hinge loss predicts: 3"
## [1] "True label: 3"
## [1] ""
# how many times did the predictions coincide?
count
## [1] 95
```